



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:19 pm BST

PDB ID : 1DN0
Title : STRUCTURE OF THE FAB FRAGMENT FROM A HUMAN IGM COLD AGGLUTININ
Authors : Cauerhff, A.; Braden, B.; Carvalho, J.G.; Leoni, J.; Polikarpov, I.; Goldbaum, F.
Deposited on : 1999-12-15
Resolution : 2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

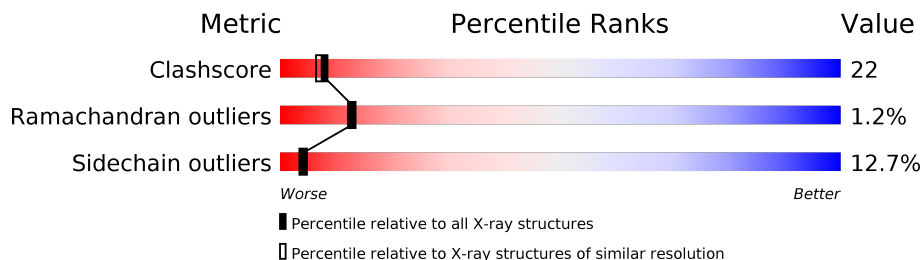
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	215	
1	C	215	
2	B	232	
2	D	232	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7208 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1638	1023	275	335	5	0	0	0
1	C	215	1638	1023	275	335	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	CYS	GLY	CONFLICT	PIR A23746
A	89	CYS	GLY	CONFLICT	PIR A23746
A	215	CYS	GLY	CONFLICT	PIR A23746
C	23	CYS	GLY	CONFLICT	PIR A23746
C	89	CYS	GLY	CONFLICT	PIR A23746
C	215	CYS	GLY	CONFLICT	PIR A23746

- Molecule 2 is a protein called IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	216	1657	1052	279	321	5	0	0	0
2	D	217	1661	1055	280	320	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLU	-	CONFLICT	PIR B23746
B	200	ALA	GLN	CONFLICT	PIR B23746
D	1	GLU	-	CONFLICT	PIR B23746
D	200	ALA	GLN	CONFLICT	PIR B23746

- Molecule 3 is water.

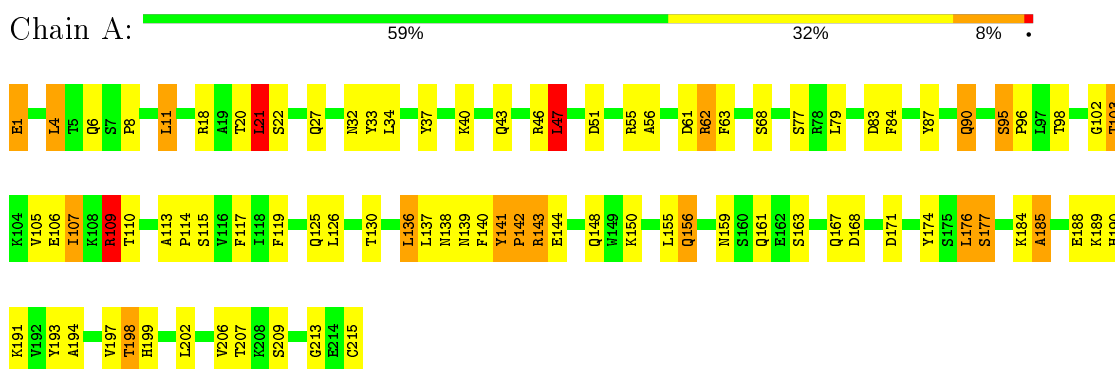
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total 163	O 163	0	0
3	B	156	Total 156	O 156	0	0
3	C	149	Total 149	O 149	0	0
3	D	146	Total 146	O 146	0	0

3 Residue-property plots

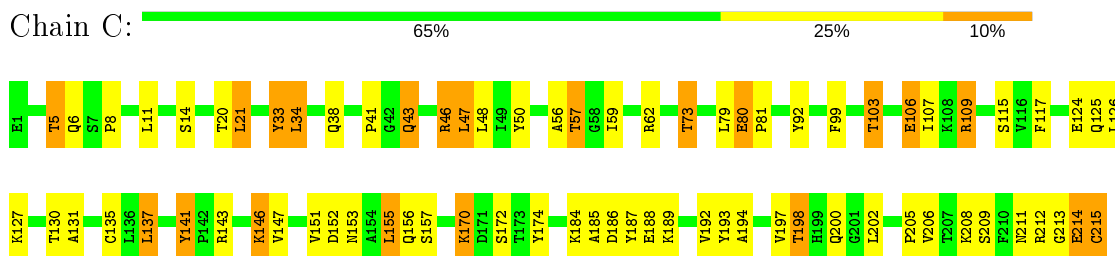
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

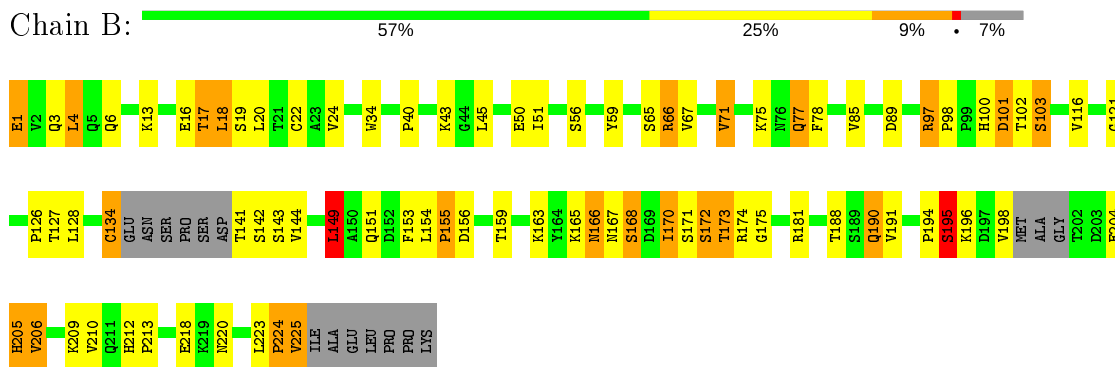
- Molecule 1: IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN)



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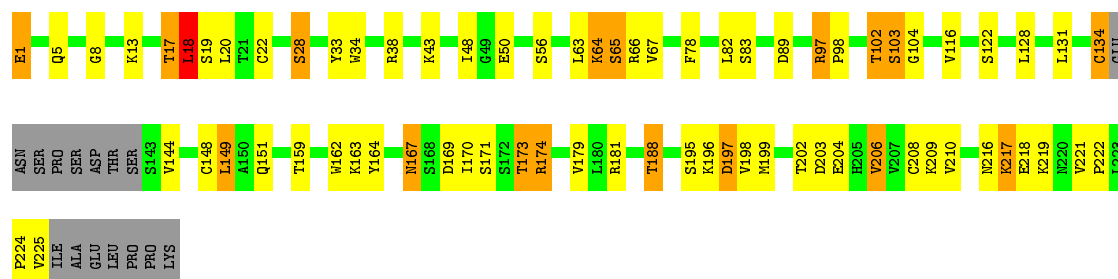


- Molecule 2: IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN)



- Molecule 2: IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN)

Chain D:  62% 24% 7% 6%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.88Å 110.88Å 170.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.28	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.28)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7208	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.09	0/1673	1.20	14/2273 (0.6%)
1	C	1.12	3/1673 (0.2%)	1.27	11/2273 (0.5%)
2	B	1.05	1/1703 (0.1%)	1.12	8/2325 (0.3%)
2	D	1.10	0/1708	1.09	3/2332 (0.1%)
All	All	1.09	4/6757 (0.1%)	1.17	36/9203 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	225	VAL	CA-CB	5.71	1.66	1.54
1	C	50	TYR	CE2-CZ	5.63	1.45	1.38
1	C	99	PHE	CE2-CZ	5.33	1.47	1.37
1	C	215	CYS	CB-SG	-5.12	1.73	1.81

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	ARG	NE-CZ-NH2	-16.46	112.07	120.30
1	A	46	ARG	NE-CZ-NH2	-13.63	113.48	120.30
1	C	62	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	C	62	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	C	46	ARG	NE-CZ-NH1	9.73	125.17	120.30
2	B	66	ARG	NE-CZ-NH2	-9.32	115.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH2	-9.05	115.77	120.30
2	B	66	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	47	LEU	CA-CB-CG	7.14	131.73	115.30
1	C	46	ARG	CG-CD-NE	-7.14	96.81	111.80
1	A	46	ARG	NE-CZ-NH1	6.75	123.67	120.30
2	B	71	VAL	CB-CA-C	-6.70	98.67	111.40
1	A	109	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	D	18	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	46	ARG	CG-CD-NE	-5.93	99.35	111.80
1	C	34	LEU	CA-CB-CG	-5.61	102.39	115.30
1	C	107	ILE	CB-CA-C	-5.59	100.42	111.60
1	A	109	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	4	LEU	CA-CB-CG	-5.53	102.57	115.30
2	B	170	ILE	N-CA-C	-5.47	96.23	111.00
1	C	43	GLN	CB-CA-C	-5.44	99.53	110.40
2	B	149	LEU	CA-CB-CG	5.38	127.68	115.30
2	D	13	LYS	CD-CE-NZ	-5.36	99.38	111.70
1	C	57	THR	CB-CA-C	-5.34	97.19	111.60
1	A	62	ARG	CG-CD-NE	-5.32	100.62	111.80
2	D	225	VAL	N-CA-C	5.25	125.17	111.00
1	C	57	THR	N-CA-CB	5.23	120.24	110.30
1	C	115	SER	N-CA-C	-5.22	96.91	111.00
1	A	21	LEU	CA-CB-CG	5.17	127.19	115.30
2	B	101	ASP	CB-CG-OD1	-5.14	113.67	118.30
2	B	175	GLY	N-CA-C	5.13	125.92	113.10
2	B	156	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	27	GLN	N-CA-C	-5.08	97.28	111.00
1	A	115	SER	N-CA-C	-5.07	97.30	111.00
1	A	51	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	106	GLU	N-CA-CB	-5.01	101.59	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TYR	Sidechain
1	A	33	TYR	Sidechain
1	C	141	TYR	Sidechain
1	C	33	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1638	0	1587	78	0
1	C	1638	0	1587	69	0
2	B	1657	0	1601	72	0
2	D	1661	0	1607	71	0
3	A	163	0	0	12	0
3	B	156	0	0	2	1
3	C	149	0	0	9	0
3	D	146	0	0	6	0
All	All	7208	0	6382	277	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (277) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLU:OE1	2:B:1:GLU:N	1.75	1.19
1:C:198:THR:HG22	3:C:2200:HOH:O	1.55	1.04
1:C:215:CYS:HB3	2:D:134:CYS:HB2	1.38	1.04
2:D:1:GLU:N	2:D:1:GLU:OE1	1.91	1.03
2:D:181:ARG:HH11	2:D:181:ARG:HB3	1.32	0.94
2:B:1:GLU:H3	2:B:1:GLU:CD	1.70	0.94
2:B:1:GLU:CD	2:B:1:GLU:N	2.17	0.94
1:A:184:LYS:O	1:A:188:GLU:HG3	1.72	0.87
2:D:181:ARG:NH1	2:D:181:ARG:HB3	1.90	0.87
2:D:181:ARG:HH11	2:D:181:ARG:CB	1.87	0.87
2:D:209:LYS:HG2	2:D:218:GLU:HG2	1.54	0.86
1:C:213:GLY:O	1:C:215:CYS:N	2.09	0.86
2:B:163:LYS:HD2	2:B:209:LYS:NZ	1.95	0.81
2:D:144:VAL:HG11	2:D:224:PRO:HG3	1.63	0.81
1:A:176:LEU:HD23	1:A:176:LEU:C	2.02	0.80
2:B:18:LEU:HD11	2:B:20:LEU:HG	1.63	0.80
2:D:18:LEU:HD22	2:D:116:VAL:HG11	1.65	0.79
1:A:198:THR:HG23	3:A:2131:HOH:O	1.83	0.78
2:B:97:ARG:HD3	2:B:98:PRO:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LEU:HD13	1:C:206:VAL:HG23	1.67	0.76
1:A:167:GLN:HG3	1:A:174:TYR:CZ	2.21	0.75
2:B:18:LEU:HD12	2:B:19:SER:N	2.01	0.74
2:B:181:ARG:HG2	3:B:2444:HOH:O	1.87	0.74
1:A:198:THR:HG21	3:A:2507:HOH:O	1.88	0.73
2:D:149:LEU:HD23	2:D:188:THR:HG22	1.69	0.73
2:B:17:THR:HG22	3:B:2138:HOH:O	1.89	0.72
2:B:166:ASN:OD1	2:B:168:SER:HB2	1.90	0.72
1:A:8:PRO:O	1:A:103:THR:HB	1.90	0.71
2:B:143:SER:HA	2:B:194:PRO:HA	1.72	0.71
1:C:8:PRO:O	1:C:103:THR:HB	1.91	0.71
2:B:34:TRP:CH2	2:B:97:ARG:HG3	2.26	0.70
2:D:1:GLU:N	2:D:1:GLU:CD	2.38	0.70
1:C:215:CYS:HB3	2:D:134:CYS:CB	2.20	0.70
1:C:153:ASN:ND2	3:C:2599:HOH:O	2.15	0.70
2:D:103:SER:HB2	3:D:2351:HOH:O	1.92	0.70
2:B:149:LEU:HD23	2:B:188:THR:HG22	1.74	0.69
2:B:18:LEU:HD22	2:B:116:VAL:HG11	1.74	0.69
1:C:143:ARG:O	1:C:143:ARG:HD2	1.92	0.69
2:D:209:LYS:HG2	2:D:218:GLU:CG	2.21	0.69
2:B:205:HIS:C	2:B:205:HIS:HD1	1.95	0.69
1:A:20:THR:HG23	3:A:2491:HOH:O	1.94	0.68
2:D:63:LEU:O	2:D:65:SER:OG	2.10	0.68
2:B:18:LEU:C	2:B:18:LEU:HD12	2.15	0.68
1:C:20:THR:HG23	3:C:2452:HOH:O	1.92	0.67
1:A:215:CYS:SG	2:B:134:CYS:CB	2.84	0.66
1:A:61:ASP:HB2	3:A:2460:HOH:O	1.96	0.66
2:B:172:SER:O	2:B:191:VAL:HA	1.96	0.66
2:D:173:THR:HG22	3:D:2576:HOH:O	1.95	0.66
2:B:142:SER:HA	2:B:195:SER:HB2	1.78	0.66
2:D:34:TRP:O	2:D:50:GLU:HA	1.96	0.66
2:B:205:HIS:C	2:B:205:HIS:ND1	2.48	0.65
2:B:40:PRO:HB2	2:B:43:LYS:HG3	1.78	0.65
1:A:37:TYR:OH	1:A:90:GLN:NE2	2.29	0.65
1:A:156:GLN:HG3	1:A:159:ASN:HD21	1.61	0.65
1:C:146:LYS:HB3	1:C:198:THR:HG23	1.78	0.65
2:B:165:LYS:HG3	2:B:205:HIS:CE1	2.31	0.64
2:B:170:ILE:HD11	2:B:206:VAL:CG2	2.26	0.64
2:B:163:LYS:HD2	2:B:209:LYS:HZ2	1.62	0.64
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.63	0.64
2:B:205:HIS:CD2	2:B:220:ASN:HB3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLU:O	2:B:85:VAL:HG22	1.99	0.62
2:D:18:LEU:HD12	2:D:19:SER:N	2.15	0.62
2:D:17:THR:HG22	3:D:2216:HOH:O	2.01	0.61
3:C:2600:HOH:O	2:D:174:ARG:HD2	2.00	0.61
1:C:192:VAL:HG22	1:C:211:ASN:OD1	2.00	0.61
2:D:34:TRP:CZ3	2:D:97:ARG:HB2	2.36	0.61
2:B:142:SER:CA	2:B:195:SER:HB2	2.31	0.61
2:B:224:PRO:O	2:B:225:VAL:HG12	2.02	0.60
1:C:33:TYR:HB3	1:C:92:TYR:CD1	2.37	0.60
1:A:114:PRO:HB3	1:A:140:PHE:HB3	1.83	0.60
1:C:188:GLU:O	1:C:212:ARG:NH2	2.35	0.60
2:D:67:VAL:HG22	2:D:82:LEU:CD1	2.32	0.60
2:B:100:HIS:HB2	2:B:103:SER:HB2	1.83	0.59
1:A:103:THR:HG21	3:A:2086:HOH:O	2.03	0.59
1:C:43:GLN:N	1:C:43:GLN:NE2	2.51	0.59
2:D:144:VAL:HG11	2:D:224:PRO:CG	2.33	0.58
2:B:1:GLU:H1	2:B:1:GLU:CD	2.04	0.58
1:C:41:PRO:O	1:C:43:GLN:NE2	2.37	0.58
1:C:170:LYS:HB3	1:C:170:LYS:NZ	2.18	0.58
1:C:198:THR:HB	1:C:205:PRO:HG3	1.84	0.58
2:D:97:ARG:HD3	2:D:98:PRO:O	2.03	0.58
1:A:18:ARG:HH21	1:A:77:SER:HB2	1.69	0.57
2:D:1:GLU:OE1	2:D:1:GLU:CA	2.53	0.57
2:B:174:ARG:HG3	2:B:190:GLN:O	2.05	0.57
1:A:159:ASN:N	1:A:159:ASN:OD1	2.37	0.56
2:D:198:VAL:HG23	2:D:199:MET:N	2.20	0.56
1:A:109:ARG:HD3	1:A:110:THR:O	2.03	0.56
1:A:167:GLN:HG3	1:A:174:TYR:OH	2.04	0.56
2:B:18:LEU:CD1	2:B:20:LEU:HG	2.36	0.56
1:A:21:LEU:HD23	1:A:21:LEU:N	2.21	0.56
1:C:5:THR:HG23	3:C:2169:HOH:O	2.06	0.56
1:A:55:ARG:NH1	3:A:2402:HOH:O	2.40	0.55
1:C:124:GLU:OE1	2:D:219:LYS:NZ	2.33	0.55
2:D:144:VAL:CG1	2:D:224:PRO:HG3	2.35	0.55
2:D:197:ASP:OD2	2:D:197:ASP:N	2.39	0.55
1:C:184:LYS:O	1:C:188:GLU:HG3	2.07	0.55
2:D:148:CYS:HB2	2:D:162:TRP:CH2	2.42	0.55
2:D:164:TYR:CZ	2:D:170:ILE:HG12	2.42	0.55
2:B:212:HIS:CG	2:B:213:PRO:HD2	2.42	0.55
1:C:143:ARG:HG2	1:C:143:ARG:NH1	2.21	0.55
1:C:80:GLU:HG3	1:C:81:PRO:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:LYS:HG3	2:B:205:HIS:HE1	1.72	0.55
2:D:128:LEU:HD21	2:D:210:VAL:HG11	1.89	0.55
1:A:206:VAL:CG1	1:A:207:THR:N	2.70	0.54
1:A:113:ALA:HB1	1:A:202:LEU:CD2	2.37	0.54
2:B:34:TRP:HB3	2:B:78:PHE:CZ	2.43	0.54
2:B:97:ARG:CD	2:B:98:PRO:O	2.54	0.54
1:C:126:LEU:HD21	1:C:131:ALA:HB2	1.90	0.53
1:A:47:LEU:HD13	1:A:56:ALA:HB2	1.89	0.53
1:A:103:THR:CG2	3:A:2086:HOH:O	2.56	0.53
2:D:216:ASN:C	2:D:217:LYS:HG2	2.28	0.53
2:D:63:LEU:HD22	2:D:82:LEU:HD11	1.91	0.53
1:A:148:GLN:HG2	1:A:155:LEU:CD2	2.39	0.53
1:A:22:SER:HB3	3:A:2264:HOH:O	2.08	0.53
2:B:170:ILE:HD11	2:B:206:VAL:HG21	1.90	0.53
1:A:215:CYS:HB2	3:A:2424:HOH:O	2.08	0.52
1:C:6:GLN:HB3	1:C:103:THR:HG22	1.90	0.52
1:C:38:GLN:HB2	1:C:48:LEU:HD11	1.91	0.52
2:D:34:TRP:HB3	2:D:78:PHE:CZ	2.44	0.52
1:A:176:LEU:CD2	1:A:176:LEU:C	2.76	0.52
2:D:159:THR:O	2:D:210:VAL:HA	2.09	0.52
1:A:189:LYS:O	1:A:190:HIS:CG	2.63	0.52
2:D:18:LEU:HD12	2:D:18:LEU:C	2.30	0.52
1:A:18:ARG:HD3	3:A:2004:HOH:O	2.10	0.52
1:A:215:CYS:SG	2:B:134:CYS:HB3	2.49	0.52
1:C:109:ARG:HD2	1:C:141:TYR:CG	2.45	0.52
2:D:144:VAL:HG13	3:D:2573:HOH:O	2.09	0.52
2:B:142:SER:HA	2:B:195:SER:CB	2.40	0.51
2:D:131:LEU:HD23	3:D:2597:HOH:O	2.09	0.51
1:A:139:ASN:HD21	2:B:174:ARG:NH2	2.09	0.51
1:C:106:GLU:HG3	1:C:174:TYR:OH	2.10	0.51
1:C:11:LEU:HD12	1:C:21:LEU:HD22	1.92	0.51
2:B:209:LYS:HE2	2:B:218:GLU:OE2	2.11	0.51
1:A:119:PHE:HE2	1:A:136:LEU:HD22	1.76	0.51
1:A:136:LEU:HD23	2:B:190:GLN:NE2	2.26	0.51
1:A:148:GLN:HG2	1:A:155:LEU:HD23	1.94	0.50
2:D:164:TYR:CE1	2:D:170:ILE:HG12	2.47	0.50
1:A:141:TYR:CD2	1:A:142:PRO:HA	2.46	0.50
2:B:209:LYS:HG2	2:B:218:GLU:HB3	1.92	0.50
1:A:156:GLN:CG	1:A:159:ASN:HD21	2.25	0.50
1:A:62:ARG:HD2	1:A:83:ASP:OD2	2.12	0.50
1:C:186:ASP:HA	1:C:189:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:LYS:HD2	2:B:209:LYS:HZ1	1.75	0.49
2:D:198:VAL:CG2	2:D:199:MET:N	2.74	0.49
1:A:87:TYR:O	1:A:102:GLY:HA2	2.12	0.49
1:A:150:LYS:HB2	1:A:194:ALA:HB3	1.93	0.49
2:B:126:PRO:HB3	2:B:153:PHE:HB3	1.94	0.49
2:D:34:TRP:HB3	2:D:78:PHE:CE1	2.47	0.49
1:A:40:LYS:HB2	1:A:43:GLN:HG3	1.94	0.49
2:D:63:LEU:HB3	2:D:67:VAL:CG2	2.43	0.49
1:A:1:GLU:HG3	1:A:98:THR:HG21	1.93	0.49
2:B:143:SER:HA	2:B:195:SER:H	1.77	0.49
2:B:34:TRP:CZ3	2:B:97:ARG:HG3	2.48	0.49
2:B:34:TRP:O	2:B:50:GLU:HA	2.11	0.49
1:A:161:GLN:OE1	2:B:181:ARG:HD3	2.13	0.48
1:A:137:LEU:HD22	1:A:197:VAL:HG21	1.95	0.48
2:B:154:LEU:HD12	2:B:155:PRO:HA	1.96	0.48
2:B:142:SER:C	2:B:195:SER:HB2	2.34	0.48
1:C:146:LYS:HE2	1:C:198:THR:CG2	2.43	0.48
2:D:38:ARG:HD3	2:D:48:ILE:HD11	1.94	0.48
2:D:163:LYS:NZ	2:D:169:ASP:OD1	2.43	0.48
2:B:170:ILE:HD11	2:B:206:VAL:HG22	1.94	0.48
2:B:205:HIS:HA	2:B:223:LEU:HG	1.95	0.47
2:D:8:GLY:HA3	2:D:20:LEU:HD23	1.96	0.47
1:C:146:LYS:HB3	1:C:146:LYS:HE2	1.74	0.47
1:C:146:LYS:NZ	1:C:198:THR:HG21	2.29	0.47
2:D:181:ARG:NH1	2:D:181:ARG:CB	2.60	0.47
1:A:37:TYR:HE2	1:A:90:GLN:HE21	1.63	0.47
2:B:170:ILE:CD1	2:B:206:VAL:HG21	2.45	0.47
1:A:119:PHE:CE2	1:A:136:LEU:HD22	2.50	0.47
2:B:13:LYS:HE3	2:B:121:GLY:O	2.15	0.47
2:D:17:THR:HB	2:D:83:SER:HA	1.95	0.47
2:B:75:LYS:HB2	2:B:77:GLN:HG3	1.97	0.46
2:B:1:GLU:OE1	2:B:1:GLU:CA	2.57	0.46
1:A:4:LEU:HA	1:A:4:LEU:HD23	1.52	0.46
1:A:125:GLN:HG2	1:A:130:THR:O	2.16	0.46
1:A:144:GLU:CD	1:A:144:GLU:H	2.19	0.46
2:B:4:LEU:HB3	2:B:22:CYS:SG	2.56	0.46
2:D:34:TRP:CZ3	2:D:97:ARG:HG3	2.49	0.46
2:D:28:SER:HB2	3:D:2376:HOH:O	2.16	0.46
1:A:18:ARG:NH2	1:A:77:SER:HB2	2.30	0.46
2:B:34:TRP:CZ3	2:B:97:ARG:HB2	2.50	0.46
2:D:34:TRP:CH2	2:D:97:ARG:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:TRP:CE3	2:D:97:ARG:HB2	2.50	0.45
1:A:6:GLN:HB3	1:A:103:THR:HG22	1.98	0.45
2:B:24:VAL:HG21	2:B:34:TRP:CH2	2.51	0.45
1:A:138:ASN:HB3	1:A:139:ASN:ND2	2.32	0.45
1:A:32:ASN:OD1	1:A:68:SER:HA	2.15	0.45
1:C:215:CYS:CB	2:D:134:CYS:SG	3.04	0.45
2:D:33:TYR:HB3	2:D:50:GLU:HB2	1.99	0.45
1:C:92:TYR:CE1	2:D:104:GLY:HA3	2.51	0.45
2:B:128:LEU:HD11	2:B:210:VAL:HG22	1.97	0.45
2:D:64:LYS:HB3	2:D:64:LYS:NZ	2.31	0.45
1:C:193:TYR:HE1	1:C:212:ARG:HG3	1.82	0.45
1:C:5:THR:CG2	3:C:2169:HOH:O	2.63	0.45
2:D:102:THR:O	2:D:103:SER:O	2.34	0.45
2:D:66:ARG:NH2	2:D:89:ASP:OD2	2.49	0.45
1:A:176:LEU:HD23	1:A:176:LEU:O	2.17	0.44
1:A:198:THR:CG2	3:A:2131:HOH:O	2.52	0.44
1:C:146:LYS:HB3	1:C:198:THR:CG2	2.45	0.44
2:D:216:ASN:O	2:D:217:LYS:HG2	2.17	0.44
2:B:212:HIS:HA	2:B:213:PRO:HD3	1.80	0.44
1:A:176:LEU:HD23	1:A:177:SER:N	2.32	0.44
1:C:109:ARG:HD2	1:C:141:TYR:CB	2.48	0.44
1:C:6:GLN:HB3	1:C:103:THR:CG2	2.47	0.44
1:C:215:CYS:CB	2:D:134:CYS:HG	2.27	0.44
1:A:107:ILE:HB	1:A:167:GLN:HE22	1.82	0.44
1:A:213:GLY:O	1:C:127:LYS:HG2	2.17	0.44
2:B:4:LEU:N	2:B:4:LEU:HD23	2.33	0.44
1:C:185:ALA:O	1:C:189:LYS:HG3	2.17	0.44
2:D:5:GLN:O	2:D:22:CYS:HA	2.18	0.44
1:A:168:ASP:HB3	1:A:171:ASP:OD1	2.18	0.43
1:C:146:LYS:CB	1:C:198:THR:HG23	2.48	0.43
1:C:48:LEU:CD2	1:C:59:ILE:HD12	2.48	0.43
2:D:1:GLU:H3	2:D:1:GLU:CD	1.92	0.43
2:B:171:SER:O	2:B:173:THR:N	2.51	0.43
2:D:66:ARG:HH22	2:D:89:ASP:CG	2.22	0.43
1:A:117:PHE:CD1	1:A:117:PHE:N	2.87	0.43
1:A:206:VAL:HG12	1:A:207:THR:N	2.32	0.43
1:A:194:ALA:HB2	1:A:209:SER:HB3	2.01	0.43
1:A:84:PHE:CD2	1:A:105:VAL:HG12	2.53	0.43
2:D:18:LEU:HD11	2:D:20:LEU:HG	2.00	0.43
1:A:43:GLN:HB2	3:A:2008:HOH:O	2.19	0.43
1:C:103:THR:CG2	3:C:2170:HOH:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:C	1:A:137:LEU:HD23	2.38	0.43
1:C:155:LEU:HD22	1:C:156:GLN:O	2.18	0.43
2:D:102:THR:HG22	2:D:103:SER:H	1.84	0.43
2:D:128:LEU:HD21	2:D:210:VAL:CG1	2.49	0.43
1:A:185:ALA:O	1:A:188:GLU:HB2	2.19	0.43
1:C:143:ARG:HD2	1:C:143:ARG:C	2.39	0.43
1:C:46:ARG:HD3	3:C:2049:HOH:O	2.19	0.43
1:C:151:VAL:HB	1:C:156:GLN:NE2	2.34	0.43
1:C:47:LEU:HD13	1:C:56:ALA:HB2	1.99	0.43
1:A:199:HIS:O	1:A:202:LEU:HB2	2.18	0.42
1:C:43:GLN:N	1:C:43:GLN:CD	2.71	0.42
2:B:59:TYR:CE2	2:B:67:VAL:HG12	2.54	0.42
1:C:137:LEU:HD22	1:C:197:VAL:HG21	2.02	0.42
2:B:3:GLN:C	2:B:4:LEU:HD23	2.39	0.42
1:C:33:TYR:HB3	1:C:92:TYR:CE1	2.54	0.42
1:C:125:GLN:HG2	1:C:130:THR:O	2.19	0.42
2:D:170:ILE:HD11	2:D:206:VAL:HG22	2.01	0.42
1:C:212:ARG:O	1:C:214:GLU:N	2.50	0.42
1:C:126:LEU:CD2	1:C:131:ALA:HB2	2.49	0.42
1:C:187:TYR:CE2	1:C:212:ARG:HD3	2.54	0.42
1:A:141:TYR:CG	1:A:142:PRO:HA	2.54	0.42
1:A:193:TYR:O	1:A:209:SER:HA	2.19	0.42
1:C:11:LEU:CD1	1:C:21:LEU:HD22	2.49	0.42
1:C:215:CYS:CB	2:D:134:CYS:HB2	2.29	0.42
1:C:109:ARG:HG2	1:C:172:SER:HB2	2.01	0.42
2:B:66:ARG:HH22	2:B:89:ASP:CG	2.23	0.41
1:C:193:TYR:O	1:C:209:SER:HB2	2.20	0.41
1:C:117:PHE:O	1:C:135:CYS:HA	2.20	0.41
1:C:147:VAL:HG22	1:C:197:VAL:HG22	2.02	0.41
1:C:194:ALA:CB	1:C:209:SER:HB3	2.51	0.41
2:D:102:THR:CG2	2:D:103:SER:N	2.84	0.41
1:A:137:LEU:CD2	1:A:197:VAL:HG21	2.51	0.41
2:B:143:SER:CA	2:B:195:SER:H	2.33	0.41
1:A:144:GLU:CD	1:A:144:GLU:N	2.74	0.41
2:B:101:ASP:OD1	2:B:102:THR:N	2.54	0.41
1:A:62:ARG:HB3	1:A:62:ARG:HE	1.62	0.41
2:B:51:ILE:HA	2:B:56:SER:O	2.21	0.41
1:A:95:SER:HA	1:A:96:PRO:HA	1.78	0.41
1:C:152:ASP:O	1:C:153:ASN:HB2	2.20	0.41
1:C:208:LYS:HA	1:C:208:LYS:HD3	1.92	0.41
2:D:221:VAL:HA	2:D:222:PRO:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HB2	1:A:174:TYR:CE1	2.55	0.40
1:C:73:THR:CG2	3:C:2538:HOH:O	2.68	0.40
2:D:209:LYS:CG	2:D:218:GLU:HG2	2.36	0.40
1:A:114:PRO:HB3	1:A:140:PHE:CD2	2.56	0.40
1:A:11:LEU:HD12	1:A:21:LEU:HD22	2.03	0.40
1:C:211:ASN:HB2	1:C:214:GLU:OE2	2.21	0.40
2:D:163:LYS:HE3	2:D:167:ASN:OD1	2.22	0.40
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.76	0.40
1:A:148:GLN:CG	1:A:155:LEU:HD21	2.51	0.40
2:B:101:ASP:OD1	2:B:102:THR:HG23	2.21	0.40
1:A:62:ARG:HG2	1:A:63:PHE:CD1	2.57	0.40
2:B:212:HIS:CD2	2:B:213:PRO:HD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2132:HOH:O	3:B:2132:HOH:O[6_555]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/215 (99%)	203 (95%)	9 (4%)	1 (0%)	29	34
1	C	213/215 (99%)	199 (93%)	13 (6%)	1 (0%)	29	34
2	B	210/232 (90%)	194 (92%)	12 (6%)	4 (2%)	8	6
2	D	213/232 (92%)	198 (93%)	11 (5%)	4 (2%)	8	6
All	All	849/894 (95%)	794 (94%)	45 (5%)	10 (1%)	13	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	172	SER
1	C	214	GLU
2	D	64	LYS
2	D	103	SER
2	D	167	ASN
2	B	195	SER
2	D	174	ARG
2	B	224	PRO
1	A	185	ALA
2	B	196	LYS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	185/185 (100%)	165 (89%)	20 (11%)	6 6
1	C	185/185 (100%)	166 (90%)	19 (10%)	7 7
2	B	187/200 (94%)	158 (84%)	29 (16%)	2 2
2	D	186/200 (93%)	160 (86%)	26 (14%)	3 3
All	All	743/770 (96%)	649 (87%)	94 (13%)	4 4

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	11	LEU
1	A	21	LEU
1	A	34	LEU
1	A	47	LEU
1	A	79	LEU
1	A	90	GLN
1	A	95	SER
1	A	103	THR
1	A	107	ILE
1	A	109	ARG
1	A	136	LEU

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Mol	Chain	Res	Type
1	A	142	PRO
1	A	143	ARG
1	A	156	GLN
1	A	163	SER
1	A	176	LEU
1	A	177	SER
1	A	191	LYS
1	A	198	THR
2	B	1	GLU
2	B	4	LEU
2	B	6	GLN
2	B	17	THR
2	B	18	LEU
2	B	45	LEU
2	B	65	SER
2	B	71	VAL
2	B	77	GLN
2	B	97	ARG
2	B	103	SER
2	B	127	THR
2	B	134	CYS
2	B	141	THR
2	B	144	VAL
2	B	149	LEU
2	B	151	GLN
2	B	155	PRO
2	B	159	THR
2	B	166	ASN
2	B	167	ASN
2	B	168	SER
2	B	173	THR
2	B	190	GLN
2	B	195	SER
2	B	198	VAL
2	B	204	GLU
2	B	205	HIS
2	B	206	VAL
1	C	5	THR
1	C	14	SER
1	C	21	LEU
1	C	34	LEU
1	C	47	LEU

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Mol	Chain	Res	Type
1	C	57	THR
1	C	73	THR
1	C	79	LEU
1	C	80	GLU
1	C	103	THR
1	C	106	GLU
1	C	109	ARG
1	C	137	LEU
1	C	146	LYS
1	C	155	LEU
1	C	157	SER
1	C	170	LYS
1	C	198	THR
1	C	200	GLN
2	D	1	GLU
2	D	17	THR
2	D	18	LEU
2	D	28	SER
2	D	43	LYS
2	D	56	SER
2	D	65	SER
2	D	97	ARG
2	D	102	THR
2	D	122	SER
2	D	134	CYS
2	D	149	LEU
2	D	151	GLN
2	D	171	SER
2	D	173	THR
2	D	179	VAL
2	D	188	THR
2	D	195	SER
2	D	196	LYS
2	D	197	ASP
2	D	202	THR
2	D	203	ASP
2	D	204	GLU
2	D	206	VAL
2	D	208	CYS
2	D	217	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	138	ASN
1	A	156	GLN
1	A	200	GLN
2	B	190	GLN
2	B	214	ASN
1	C	43	GLN
2	D	76	ASN
2	D	151	GLN
2	D	205	HIS
2	D	214	ASN
2	D	220	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.